

Deformation twins in nanocrystalline Al

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Due to its high stacking fault energy, no deformation twin has ever been observed in coarse-grained Al. Recent molecular dynamic (MD) simulations predicted the formation of deformation twins in nanocrystalline (nc) Al. Here, we report transmission-electron-microscopic observations of two types of twins in nc Al processed by cryogenic ball milling. They were formed via mechanisms suggested by the MD simulations. We also observed curved twin boundaries caused by partial dislocations. These results indicate that deformation mechanisms not accessible to coarse-grained Al are active in nc Al. They could be responsible for some unique mechanical properties of nc materials. © 2003 American Institute of Physics. [DOI: 10.1063/1.1633975]

Nanocrystalline (nc) materials possess superior mechanical properties such as high strength, which sometimes coexists with very good ductility.^{1–4} These superior mechanical properties are attributed to their unique deformation mechanisms.⁵ Only recently has the scientific community begun to understand some of the deformation mechanisms that operate in nc materials.^{6–12} For example, molecular dynamic (MD) simulations have predicted deformation twinning in nc fcc Al,^{12,13} which was very surprising because no deformation twin has ever been observed in coarse-grained Al due to its high stacking fault energy. The deformation twins were recently confirmed in nc Al film produced by physical vapor deposition.¹⁴ However, the twinning mechanisms were not very clear. Our recent study on nc Al produced by cryogenic ball milling¹⁵ revealed that deformation twins could form via the dynamic overlapping of stacking fault ribbons formed by Shockley partial dislocations emitted from grain boundaries (GBs), which is consistent with the homogeneous twinning mechanism predicted by MD simulations.^{12,13} The MD simulation also predicted two other twinning mechanisms:¹³ (i) heterogeneous twins nucleated from GBs and (ii) twin lamellae via the dissociation and migration of GBs. However, twins formed via these two mechanisms have not been experimentally confirmed. In this letter, we report a further study on twinning in nc Al processed by cryogenic ball milling and the observation of twins formed by the latter two mechanisms predicted by MD simulations.

Al powder with a purity of ~99.9 wt % was ball milled while immersed in liquid nitrogen. Readers are referred to Ref. 15 for more details. The as-milled Al powder contains both elongated and equiaxed grains.¹⁵ The diameters of most equiaxed grains and the widths of most elongated grains are smaller than 100 nm. Figure 1 shows (a) a transmission electron microscopy (TEM) micrograph of a twin at the lower

corner of a grain with the twin boundary marked by two white arrows, and (b) a high-resolution TEM (HRTEM) image of the twin. The twin was likely formed by the heterogeneous mechanism proposed by Yamakov *et al.*¹³ Specifically, the twin was likely nucleated at the lower corner of the grain and grew larger via the emission of Shockley partial dislocations from the GB. As shown, the whole lower corner below the twin boundary has been transformed into a twin. It is not clear if the first partial dislocation was emitted at the very bottom of the corner, but further growth of the twin shown in Fig. 1 can only occur by partial dislocation emission at a plane above and adjacent to the twin boundary, which moves the twin boundary upward. MD simulations indicate that at very fine grain sizes (e.g., <8 nm), GB slid-

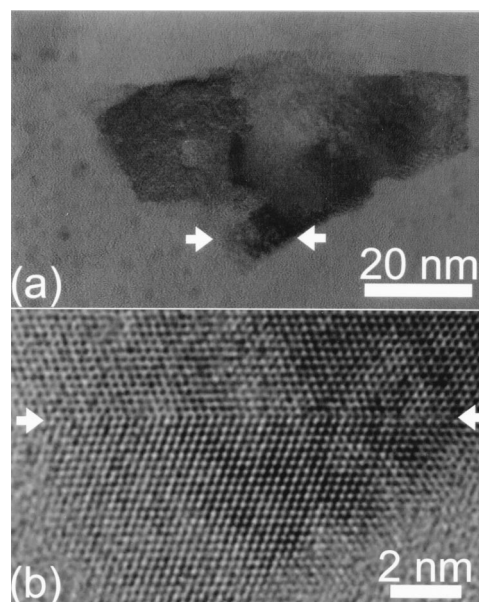


FIG. 1. (a) A deformation twin at the lower corner of a large grain with the twin boundaries marked by two white arrows, and (b) HRTEM image of the twin.

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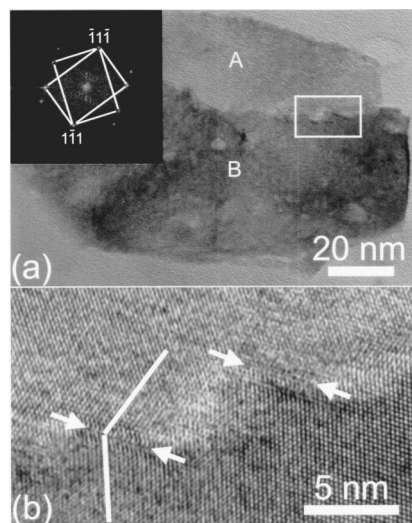


FIG. 2. (a) Areas A and B form a twinning relationship with a wavy boundary between them. The inset shows Fourier transformation of a region that encompasses areas A and B, which indicates a $(\bar{1}\bar{1}1)$ twinning plane; (b) HRTEM image of a twin boundary segment from the white frame in (a). It consists of short, straight, coherent (111) twinning planes (marked by arrows) connected by incoherent, noncrystallographic segments.

ing and GB diffusion are the primary deformation mechanisms.^{6,7,11} At larger grain sizes (e.g., 8–45 nm), partial dislocations emitted from GBs contribute significantly to the deformation.^{10–13,15–17} The MD simulations usually predict very high critical shear stresses of a few gigapascal for partial dislocations to emit from GBs, because of very high strain rates used in MD simulations. However, a recent analytical model¹⁸ predicted much lower critical shear stresses of a few hundred megapascal at lower strain rates that are closer to the experimental conditions of ball milling. Below 15 nm the model¹⁸ indicates that partial dislocations are emitted at a stress lower than the stress needed for emitting full dislocations. Therefore, partial dislocation emission from GBs is a viable deformation mechanism under the ball-milling conditions in this study.

Note that the twin in Fig. 1 is located at a small corner of a much larger grain of several tens of nanometers. According to the MD simulations,^{6,11,13} it would be very difficult for this grain to slide against another grain because of its large size, and partial dislocation emission from GBs is a major deformation mechanism. On the other hand, the twin boundary has a length of 14 nm, which is also the length of the slip plane. The slip plane length determines whether a partial or full dislocation is emitted from the GB.¹⁵ As the lengths of all slip planes below the twin boundary in Fig. 1(b) are shorter than 14 nm, the partial dislocation emission from GBs was the primary deformation mode. Therefore, it is logical to conclude that the twin in Fig. 1 was formed by the successive emission of partial Shockley dislocations from GBs on adjacent slip planes.

Figure 2(a) shows another type of twin. The inset in Fig. 2(a) shows the Fourier transformation of a region that encompasses areas A and B. It demonstrates that the two areas form a crystallographic twinning relationship with $(\bar{1}\bar{1}1)$ as the twinning plane. However, the boundary between area A and area B is wavy instead of the usual straight twinning plane characteristic of conventional twins. In fact, sharp,

straight boundaries are the features that are often used to identify twins in a low magnification TEM micrograph or optical photograph.

Figure 2(b) is an atomic scale image of the twinning boundary enlarged from the white frame in Fig. 2(a). It indicates that areas A and B indeed form a twin relationship. Some segments of the boundary are straight, coherent $(\bar{1}\bar{1}1)$ twin boundaries as indicated by white arrows. These segments, which are connected by noncrystallographic segments, form a zigzag boundary between the two twinning areas. Examination of the local twinning morphology in Fig. 2(b) reveals that the twin strikingly resembles a type of twin observed in the MD simulation.¹³ This type of twins is formed by an entirely different mechanism, which involves the splitting and subsequent migration of a GB segment, leaving behind two coherent twin boundaries. This mechanism was first proposed by Ashby and Harper¹⁹ in 1967 and was subsequently discussed by Gleiter.²⁰ It appears that the twin shown in Fig. 2 was formed by this mechanism. More specifically, a GB segment was dissociated into a twin boundary and a new GB.¹³ A twin lamella was formed via the migration of the new GB. The boundaries of twin lamellae formed at different time frames joined together to form the zigzag boundary between areas A and B. The noncrystallographic segments observed here were actually the new GBs in this mechanism. Readers are referred to the work by Yamaakov *et al.*¹³ for more detailed description on the twinning mechanism.

Figure 3 shows an elongated grain (with GB highlighted by dashed lines) containing two twins whose boundaries are marked by white arrows and asterisks. The inset is an HRTEM image showing the twin relationship along a twin boundary near A. The twin boundary marked as a-a has two straight segments, which are connected by a noncrystallographic segment. This twin boundary and related twin were likely formed via the same mechanism as the twin in Fig. 2. The twin boundary marked as b-b is relatively straight with a slight curvature. Similar twin boundaries were also observed in a cryogenically ball-milled Al–Mg alloy powder.²¹ The small curvature is caused by extrinsic Frank partial dislocations as well as Shockley partial dislocations in the otherwise straight (111) twin boundaries.^{21,22}

Another possible way to produce wavy twin boundary is the further deformation of a twin either formed by earlier stage deformation or formed by a possible but very small chance of two Al power particles happened to be in a twin relationship before the ball milling. The curved twin boundary b-b in Fig. 3 could be formed by this mechanism. However, it is hard to imagine how such a mechanism can form the zigzag twin boundary in Fig. 2. The coherent $(\bar{1}\bar{1}1)$ twin planes in Fig. 2 are arranged in a parallel, orderly way, which is consistent with the twin lamellae formation by GB dissociation and migration mechanism predicted by the MD simulation,¹³ instead of the random waviness that is likely produced by the further deformation of an already formed twin.

It is remarkable that all three twinning mechanisms predicted by MD simulation¹³ were verified in our TEM observation of cryogenically-ball-milled Al powder, considering the significant differences in deformation conditions in our

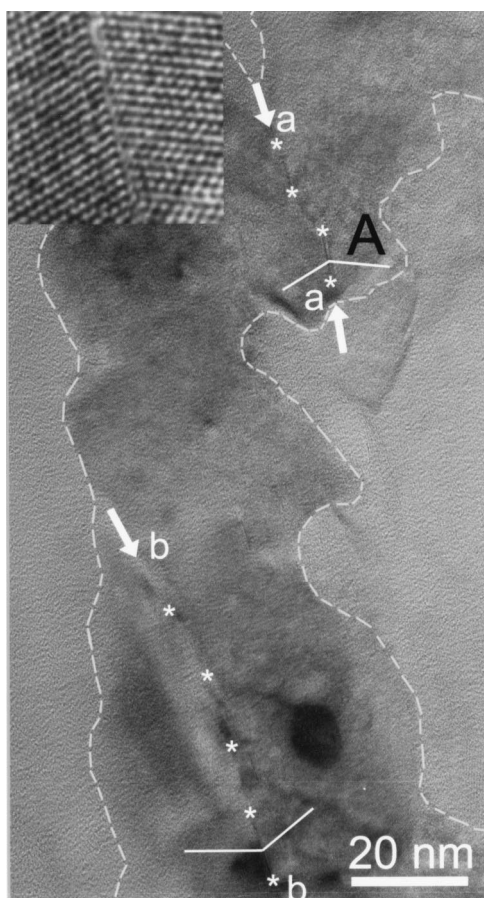


FIG. 3. An elongated grain (with GB marked by white dashed lines) containing two twin boundaries, marked by white arrows and asterisks. The inset shows the twinning relationship along a twin boundary near A. The twin boundary a-a is similar to that in Fig. 2, and the twin boundary b-b is slightly curved.

experiment¹⁵ and the MD simulation.¹³ Room temperature and extremely high strain rate (2×10^8) were used in the MD simulation.¹³ The strain rate during our cryogenic ball milling is unknown, but we believe it was several orders of magnitude lower than in the MD simulation. Both high strain rate and low temperature are known to promote twinning.²³ Therefore, the low temperature in our experiment (-196°C) compensated, to some extent, for its low strain rate in promoting deformation twinning. We also noticed that the deformation twins in our cryogenically ball-milled Al are not as prevalent as predicted by the MD simulation,¹³ which is likely due to the differences in deformation conditions.

In summary, we report the experimental observations of two types of deformation twins in cryogenically ball-milled nc Al. These observations directly verify two of the three twinning mechanisms predicted by the MD simulation,¹³ i.e.,

the heterogeneous nucleation and growth from GBs, and the twin lamella formation via the dissociation and migration of GB segments. The third twinning mechanism predicted by the MD simulation,¹³ homogeneous nucleation of twins inside grains by the dynamic overlapping of stacking faults, has been verified in our previous work.¹⁵ These twinning mechanisms are different from the conventional pole mechanisms and proved that nc Al indeed deforms via mechanisms not available in coarse-grained Al.

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